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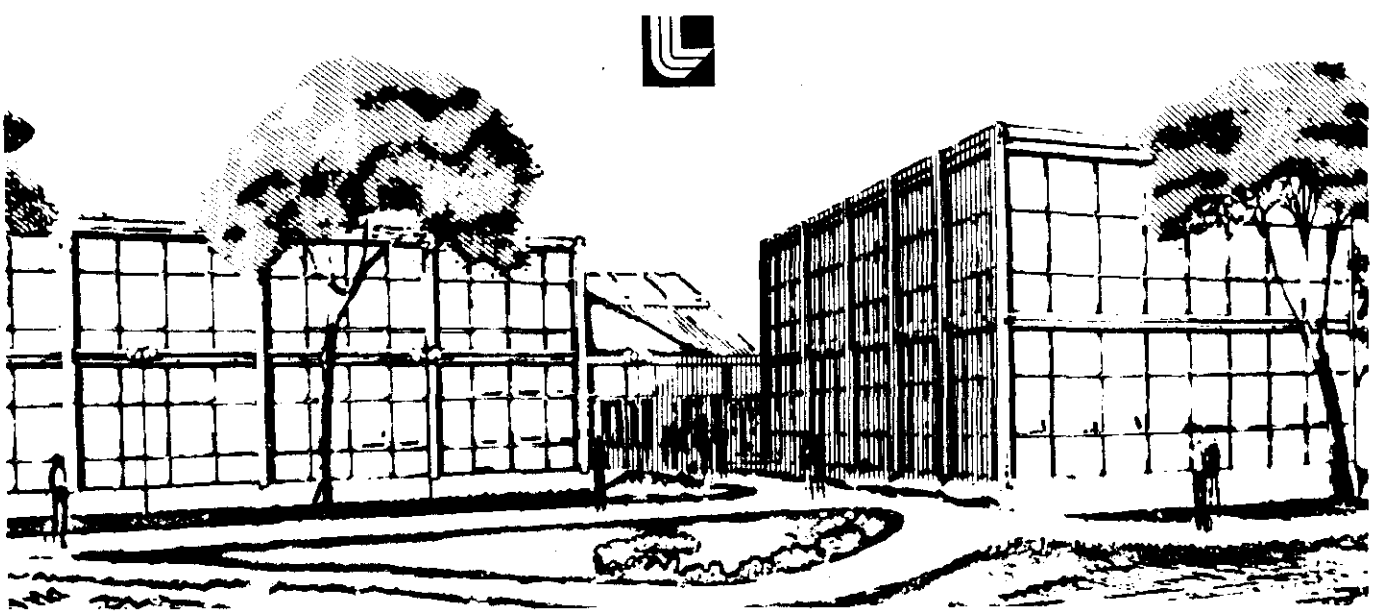

LIMITS OF THERMODYNAMIC MODELS FOR NUCLEAR LEVEL DENSITIES*

S. M. Grimes
Lawrence Livermore Laboratory
Livermore, California 94550

ABSTRACT

The current status of thermodynamic models as applied to nuclear level densities is reviewed. Considerable refinement has taken place during the last fifteen years, with the result that some of the undesirable assumptions originally required by the model are no longer necessary. Some problems remain, however, particularly in calculating level densities for deformed nuclei. Furthermore, some related parameters, such as the positive-parity negative-parity ratio for levels and the spin cutoff parameter are more sensitive to the presence of two-body interactions than the total level density. Improvement in our characterization of nuclear level densities will require use of techniques which can incorporate the effects of two body interactions in the level density calculation.

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I. INTRODUCTION

Much of the experimental and theoretical work in the field of nuclear level densities is based on the Fermi gas model. Bethe[1] introduced this model, which treats the nucleus as a group of non-interacting Fermions. They are assumed to have a single particle spectrum with a density which is independent of energy. If the grand partition function is used to express the level density in terms of integrals which are functions of the single particle energies, the thermodynamic temperature and the neutron and proton number of the nucleus, the saddle point technique can be used to carry out the integration. With these assumptions, it may be shown that the nuclear level density has an analytical form: $\rho(E) \propto e^{2\sqrt{aE}}/E^{5/4}$ where a is proportional to the density of single particle states and E is the excitation energy.

Objection might be raised to this approach, in that no allowance is made for the shell structure of nuclei and no difference in level density between even- and odd-mass nuclei is predicted. In practice, experimentalists have typically reduced the excitation energy by an amount roughly equal to the pairing gap for even A nuclei when using the above formula, thus achieving an even-A odd-A level density difference as is seen experimentally. Shell effects have been introduced into level density calculations by modifying either E or a or possibly both.

Later work with the Fermi gas model utilized levels of various degeneracies (as would occur in the spherical shell model without two-body interactions). Beginning with Rosenzweig,[2] investigations of the effects

of shell structure on Fermi gas level density calculations have been made by numerous authors.[3-7] In general, the results have indicated that for periodic single particle level schemes, the original Fermi gas level density formula is appropriate, but some adjustment is required in the excitation energy to account for shell effects.

The basic assumption of the Fermi gas model is that two-body forces may be ignored in calculating level densities. Because pairing forces have such obvious effects on the low-lying level spectrum, it is clear that the traditional Fermi gas calculation would not be reliable at low excitation energy. Use of the formalism[8] for a superconducting system allows the inclusion of pairing effects in a one-body approach.[9-11] The single particle state energies are replaced by quasi-particle energies obtained by solving the BCS equation.[8] Calculations using this model yield a level density which has roughly a constant temperature energy dependence at low energies but returns to the traditional Fermi gas form at higher energies. Even above the transition point (where the superconductivity disappears) there will remain a constant energy shift relative to the corresponding calculation without pairing. Thus, as in the case of shell effects, there is justification for introducing energy shifts in the level density expression.

The assumption that the single particle state density is either constant or periodic is required in order to obtain an analytic expression for the level density. Numerical values for the level density at specific energies can be obtained if a computer is used to evaluate the equation for the grand partition function with specific single particle

energies used in the sums.[12-14] This modification is of particular importance in that it allows shell effects to be incorporated in the calculation in a natural way. Calculations of level densities in this fashion[15,16,17] have been found to agree fairly well with data for appropriate choice of single particle energies.

II. FORMALISM OF THE FERMI GAS MODEL

Pairing effects, as indicated above, can be included in the model with the use of the BCS formalism.[8] The Hamiltonian of the system is written

$$H = \sum_k e_k \left(a_k^+ \; a_k + a_{-k}^+ \, a_{-k}\right) - G \sum_{kk'} a_{k'}^+ \, a_{-k'}^+ \, a_k \, a_{-k} \qquad (1)$$

where e_k is the energy of the $k^{\underline{th}}$ doubly degenerate energy level and $a_{\pm k}^+$ and $a_{\pm k}$ are the creation and annihilation operators for particles with spin projections + or -. G is the pairing matrix element. The grand partition function of such a system can be written

$$\begin{aligned} \Omega = & -\beta \sum_k (e_k - \lambda - E_k) \\ & +2 \sum_k \ln \left[1 + \exp(-\beta E_k)\right] \\ & -\beta \Delta^2 / G \end{aligned} \qquad (2)$$

where Δ is the energy gap, $E_k = \sqrt{(e_k - \lambda)^2 + \Delta^2}$, β is the reciprocal of the temperature and λ is the chemical potential (Fermi energy) of the system. For a given value of the temperature, one first solves the system of equations

$$\frac{2}{G} = \sum_{k_N} \frac{\tanh\left(\frac{1}{2}\beta E_{k_N}\right)}{E_{k_N}}$$

$$\frac{2}{G} = \sum_{k_Z} \frac{\tanh\left(\frac{1}{2}\beta E_{k_Z}\right)}{E_{k_Z}} \tag{3}$$

$$N = \sum_{k_N} \left[1 - \frac{(e_{k_N} - \lambda_N)}{E_{k_N}} \tanh\left(\frac{1}{2}\beta E_{k_N}\right)\right]$$

$$Z = \sum_{k_Z} \left[1 - \frac{(e_{k_Z} - \lambda_Z)}{E_{k_Z}} \tanh\left(\frac{1}{2}\beta E_{k_Z}\right)\right] \tag{4}$$

where k_N and k_Z denote sums over neutron and proton orbitals and N and Z are the neutron and proton number of the nucleus respectively; this yields values of λ and Δ for each type of nucleon. The energy of the system is given by the expression

$$E = \sum_{k_N} e_{k_N} \left[1 - \frac{e_{k_N} - \lambda_n}{E_{k_N}} \tanh\left(\frac{1}{2}\beta E_{k_N}\right)\right]$$

$$- \frac{\Delta_N^2}{G} + \sum_{k_Z} e_{k_Z} \left[1 - \frac{e_{k_Z} - \lambda_Z}{E_{k_Z}} \tanh\left(\frac{1}{2}\beta E_{k_Z}\right)\right] - \frac{\Delta_Z^2}{G} \tag{5}$$

Finally, the state density is given by

$$\rho(E,N,Z) = \frac{1}{(2\pi i)^3} \oint d\beta \oint d\alpha_N \oint d\alpha_Z e^S \tag{6}$$

where $S = \Omega_N + \Omega_Z + \beta E - \alpha_N N - \alpha_Z Z$

and α_N and α_Z are $\beta\lambda_N$ and $\beta\lambda_Z$, respectively.

Use of the saddle point procedure then gives the following value for the integral

$$\rho(E) = \frac{e^S}{(2\pi)^{3/2} D^{1/2}} \tag{7}$$

where

$$D = \begin{vmatrix} \frac{\partial^2\Omega}{\partial\alpha_N^2} & \frac{\partial^2\Omega}{\partial\alpha_N\partial\alpha_Z} & \frac{\partial^2\Omega}{\partial\alpha_N\partial\beta} \\ \frac{\partial^2\Omega}{\partial\alpha_N\partial\alpha_Z} & \frac{\partial^2\Omega}{\partial\alpha_Z^2} & \frac{\partial^2\Omega}{\partial\alpha_Z\partial\beta} \\ \frac{\partial^2\Omega}{\partial\alpha_N\partial\beta} & \frac{\partial^2\Omega}{\partial\alpha_Z\partial\beta} & \frac{\partial^2\Omega}{\partial\beta^2} \end{vmatrix}$$

The spin cutoff parameter σ is given by

$$\sigma^2 = \sigma_Z^2 + \sigma_N^2 \tag{8}$$

and $$\sigma_N^2 = \frac{1}{2}\sum_{k_N} \frac{m_{k_N}^2}{\cosh^2(\frac{1}{2}\beta E_{k_N})} \quad \text{and} \quad \sigma_Z^2 = \frac{1}{2}\sum_{k_Z} \frac{m_{k_Z}^2}{\cosh^2(\frac{1}{2}\beta E_{k_Z})}$$

and m_k is the angular momentum projection for the $k^{\underline{th}}$ level.

We then use the usual relation between level and state densities[18] to obtain the following equation for the level density $\rho(E,J)$ of levels of spin J and energy E:

$$\rho(E,J) = \frac{(2J+1)}{2(2\pi)^{\frac{1}{2}}\sigma^3}\rho(E)\exp\left[-\frac{(J+\frac{1}{2})^2}{2\sigma^2}\right] \tag{9}$$

Obtaining the energy dependence of the level density simply requires incrementing the thermodynamic temperature a number of times and repeating the calculation for each value. This formalism has been discussed in detail by Moretto[13] and has been used by various authors[12-16] for the calculation of level densities.

III. EXPERIMENTAL RESULTS AND COMPILATIONS

Nearly all of the level density information obtained to date has been interpreted in terms of the Fermi gas model. Thus, in principle, a direct comparison of a values and energy shifts should allow a comparison of the results of various measurements. In practice, the situation is not so straightforward.

Level density information comes from the use of two different procedures: 1) counting levels and 2) measuring evaporation spectra. In each case, additional assumptions made by those analyzing the data can affect the parameter values deduced from the data.

Much of the variation is due to the use of different forms for the Fermi gas level density expression. The form for the density of states[17] for the equidistant model is

$$\rho(E) = \frac{\sqrt{\pi}}{12} \frac{\exp 2\sqrt{aE}}{a^{1/4}E^{5/4}} \tag{10}$$

From Eq. (9) we see that relating $\rho(E)$ to $\rho(E,J)$ involves the spin cutoff parameter σ; by summing Eq. (9) over J we can show that

$$\sum_J \rho(E,J) = W(E) = \frac{\rho(E)}{\sqrt{2\pi}\,\sigma} \tag{11}$$

The traditional Fermi gas energy dependence for σ is $\sigma \propto E^{1/4}$, so an energy dependence of $\frac{e^{2\sqrt{aE}}}{E^{3/2}}$ is expected for W(E) and $\frac{e^{2\sqrt{aE}}}{E^2}$ is expected for $\rho(E,J)$.

Thus, depending on whether levels with a fixed number of spins are observed or all spins are seen, the energy dependence of the level density will differ. Moreover, in some cases, only the shape of the level density has been fit while in other analyses the absolute value has been included as well.

Some indication of the problems which can arise is given in Fig. 1. Level density parameters which have been proposed in four compilations[7,19-21] are compared. These compilations have all been based on neutron resonance counting, so the differences are not principally due to experimental discrepancies. Most likely, the difficulties involve the assumptions made in the analysis.

As an example, consider the analysis of Gilbert and Cameron.[19] These authors utilized the level density information obtained from low energy neutron resonances to infer the level density parameters. These data normally yield the level density for levels of only one parity and one or two J values. Consequently, one obtains a level density value at a specific energy but no information on the slope. The two parameter Fermi gas level density form is therefore underdetermined in this analysis. Gilbert and Cameron made the assumption that pairing effects would be incorporated into an energy shift, but that shell effects would only influence a and not E. This is almost certainly incorrect. We normally would anticipate that shell effects would disappear as we raise the energy to values of 30 - 50 MeV. If shell effects are incorporated into a, the reduction in level density will remain at arbitrarily large energy, while if the adjustment is in E, the level density for closed-shell nuclei will approach that for non-closed-shell nuclei at high energies. This discussion presumes, of course, that the level density for closed-shell nuclei can be expressed by the traditional Fermi gas form; this point will be discussed in more detail later. The analyses of Ref. 7 and Ref. 20 also fixed the energy shift and varied only a; Ref. 21, on the other hand, varied both a and the energy shift.

Fig. 2 illustrates the possible consequences of fitting the level density at one energy to determine the two parameters of the Fermi gas level density form. The two choices of level density parameters yield the same level density at 7 MeV, but do not agree at any other energy. Variation of a by one unit corresponds roughly to the range of values shown on Fig. 1 for a specific nucleus; note that this corresponds to a variation of about 50% at 10 MeV, even though the two calculations agree at 7 MeV.

Other level density analyses[22,23] have been based on level counting but have used various reactions to populate the levels. While there is the possibility of missed levels (this can happen in the neutron resonance analysis also), these studies have the important advantage that the energy dependence of the level density can be studied and the two parameters of the Fermi gas model better determined than from a measurement of the level density at only one energy. Finally, use of a wider range of reactions at least potentially would yield information on the level density for a number of J values and hence lead to information about the spin-cutoff parameters as well.

As the level density increases, the levels begin to overlap, so at some energy counting levels becomes impossible. In this region level densities are inferred from evaporation spectra. Use of this technique is also possible in the resolved level region, if data are taken with poor energy resolution.

Many of the inconsistencies in level density parameters deduced from evaporation spectra are due to use of the Weisskopf expression in analyzing the data. According to Weisskopf and Ewing,[24] the cross section for evaporation of a particle of energy ε can be written

$$\sigma(\varepsilon) \propto \varepsilon\sigma_{inv}(\varepsilon)\,\rho(U)$$

where $\sigma_{inv}(\varepsilon)$ is the cross section for formation of the compound nucleus by the inverse reaction and $\rho(U)$ is the level density at the excitation U of the residual nucleus and U is the excitation energy of the residual nucleus. The derivation of this result requires the assumption that the nuclear moment-of-inertia is infinite, or equivalently, that the branching ratio for decay into various channels is independent of the spin and parity of the compound state. Although these conditions clearly are not strictly fulfilled, the simplicity of the Weisskopf formalism has induced many authors to use this approach in the analysis of evaporation spectra. As a consequence, the level density parameters deduced from some of these measurements are probably unrealistic. A detailed comparison of the results of a Weisskopf analysis with the more accurate Hauser-Feshbach[25] formalism has been presented by Lu, Vaz and Huizenga.[26]

A further problem with the evaporation spectra analysis is that only the shape of the level density function is determined, without yielding an absolute normalization. If level density parameters are derived which fit a given set of emission spectra, then level density parameters which doubled the level density in all exit channels would yield the same calculated cross sections. In fact, because level density parameter changes affect both the energy dependence and magnitude of the level density, substantial variation in level density parameters is not allowed, but the determination of absolute level density values with emission spectra is not as precise as can be obtained at lower energies by level counting.

As this summary indicates, the most reliable approach to level-density-parameter compilation would be to combine the information obtained from level counting with that from evaporation spectra. At higher energies, level density determinations may be made from Ericson fluctuation measurements and inclusion of these results can also make parameter determination more reliable.

Since the bulk of the experimental level density information has been parameterized in terms of the Fermi gas model, it is interesting to determine the extent to which this form fits the calculations with realistic single particle level spacings and including pairing. Examples of comparisons are shown in Figs. 3 and 4, where the single particle levels are taken from Nilsson[27] and from Seeger and Perisho.[28] As these figures indicate, generally good agreement is found for appropriate choice of parameters. In some cases, the fit to the traditional Fermi gas form is not good below 4 or 5 MeV in excitation.

If we argue that spectral distribution calculations would represent an alternative and presumably improved approach to level density calculations, the question of how similar the energy dependence for spectral distribution calculations is to that of the traditional Fermi gas form is then of interest. Fig. 5 shows that for appropriate choice of parameters the two forms yield very similar energy dependences. Clearly, one must have a basis large enough so that the number of levels is sufficiently large, but within this constraint, appropriate choice of width and centroid yield good agreement between the two forms.

IV. LIMITATIONS OF THE FERMI GAS MODEL

The discussion to this point has indicated that the traditional Fermi gas formula can represent both the data and theoretical calculations utilizing realistic single particle schemes. While questions would remain as to the best single particle set to use, it appears that for many nuclei an optimum choice would yield good results.

An exception to this statement must be made for nuclei which are highly collective. The Fermi gas model, because it treats the nucleons as non-interacting, does not predict low-lying collective states. Consequently, level densities for deformed nuclei would be significantly underestimated. Efforts[29] have been made to remedy this omission by adding ad hoc levels corresponding to rotational bands. While this procedure represents a step in the proper direction, it is a technique which cannot be carried out self consistently. First, the levels which are added should be removed from the higher energy spectrum, since the effect of two body forces is not to create extra levels, but to lower the energy of certain levels. If one is interested in the level density only at very low energies, this procedure is defensible, but would involve difficulties at higher energies, where the cumulative effect of building additional bands on states which should have been removed from the spectrum will likely be substantial. An additional objection to this procedure is that we have a limited knowledge of how the deformation changes over a wide range of excitation energy. The results of Moretto[30] suggest that the average deformation for deformed nuclei tends to zero at high excitation energies (50-60 MeV); this result is plausible, since at high energies one would expect deformed and spherical nuclei to become similar in their nuclear properties. In both cases, there is most likely a range of deformations at higher energies. Both because of this range of deformations and because nuclei with different deformations will approach the spherical limit at different rates as a function of energy, it is difficult to justify a level density model with ad hoc deformation parameters. It has been shown, however, that inclusion of the rotational bands does produce better agreement between experiment and calculation at energies of about 7 MeV, so the difficulties with this approach apparently do not cause problems until somewhat higher energies.

These points are of particular importance in the use of level density compilation systematics to extrapolate to obtain parameters for nuclei off the stability line. Because some of these nuclei will be deformed even if the neighboring nuclei on the stability line are not, these extrapolations could be in error.

A comparison of Fermi gas model predictions for the spin cutoff parameter (σ) and the positive-negative parity ratio with data is more difficult because of the lack of measurements of these quantities. In two recent papers[15,16] spin cutoff parameters have been calculated and compared with data; the agreement is fair. The trend in σ from nucleus to nucleus is well reproduced, but, at least in the $f_{7/2}$ shell, the energy dependence of the calculated values has a systematic tendency to be too rapid. An example of such a calculation is shown in Fig. 6.

Similarly, few measured values of the positive-negative parity ratio are available. Studies of proton resonances[31] at low energy yield values for this ratio at a few MeV of excitation and indicate that this ratio is not yet unity at these energies, but definitive results at higher energies are not available. As can be seen from Fig. 7, the thermodynamic calculations of this ratio[32] are quite sensitive to choice of single particle basis, with some choices yielding results which are clearly incorrect. For heavier nuclei ($A > 70$), there is apparently a tendency[32] for thermodynamic calculations based on reasonable single particle schemes to yield equal fractions of positive and negative parity levels at excitation energies which are too low.

The cause for this discrepancy is easy to understand. It is sufficient to focus only on the negative parity orbitals, since a positive parity orbital does not change the parity of the system when occupied. If a negative parity orbital is near the Fermi level, it will have an occupation probability of about .5. Such a probability for even one negative parity orbital is sufficient to essentially balance the two parities, even if all other orbitals were of the same parity. The inclusion of pairing greatly reduces the probability of having only one of a pair $(m_Z,-m_Z)$ of orbitals occupied and thus keeps the ratio from being balanced. For heavy nuclei, however, the pairing gap vanishes at energies above 4-6 MeV and the parities are predicted to be equally likely at this point. Unfortunately, in most cases the experimental results contradict this prediction. Presumably, better agreement with experiment would result if two-body forces were included in the calculation.

V. SUMMARY

A review of recent experimental and theoretical work utilizing the Fermi gas model to characterize nuclear level densities has been presented. The use of modern high-speed computers to solve the statistical mechanical equations allows a relaxation of assumptions originally imposed to yield an analytic solution. Both pairing and shell effects appear to emerge naturally in calculations utilizing realistic single particle schemes. Although agreement between theory and experiment is good in many cases, it is argued that the Fermi gas approach will likely be unreliable for nuclei which are deformed. There are also some indications that the Fermi gas model incorrectly predicts parity ratios and spin cutoff parameters, even in situations where the level density parameters are correctly predicted. Spectral distribution methods will be particularly useful in investigating these discrepancies.

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FIGURE CAPTIONS

Fig. 1: Level density parameters deduced for Ti and Ni from neutron resonance spectroscopy. Points denoted Δ, ·, □ and x are from Refs. 7, 19, 20 and 21, respectively.

Fig. 2: Level density calculated from the Fermi gas form for two sets of parameters which yield the same value at 7 MeV. Note the divergence at lower and higher energies.

Fig. 3: Level density for ^{52}Cr as calculated from the single particle levels of Nilsson[27] and Seeger and Perisho.[28] Also shown are Fermi gas fits to the numerical calculations.

Fig. 4: Same as Fig. 3 for ^{58}Ni.

Fig. 5: Fits of the Gaussian form with two sets of parameters to the standard Fermi gas formula. The fit with the largest dimensionality provides a fit over the widest range of energy, but in both cases the agreement is quite good over a range of at least 9 MeV.

Fig. 6: Comparison of measured values for the square of the spin cutoff parameter (Ref. 16) for ^{61}Ni with thermodynamic calculations of this quantity. Note that for both sets of single particle levels the energy dependence is too rapid.

Fig. 7: Calculated positive parity-negative-parity ratios for ^{28}Si and ^{38}Ar. This parameter, $\rho^{+}(E)/(\rho^{+}(E) + \rho^{-}(E))$, tends to .5 at large energies, but would not be expected to converge to this value at energies as low as 6 MeV (for an even-even nucleus). The calculations indicated -· and -- are based on single particle energies proposed in Ref. 27 and Ref. 28, respectively.

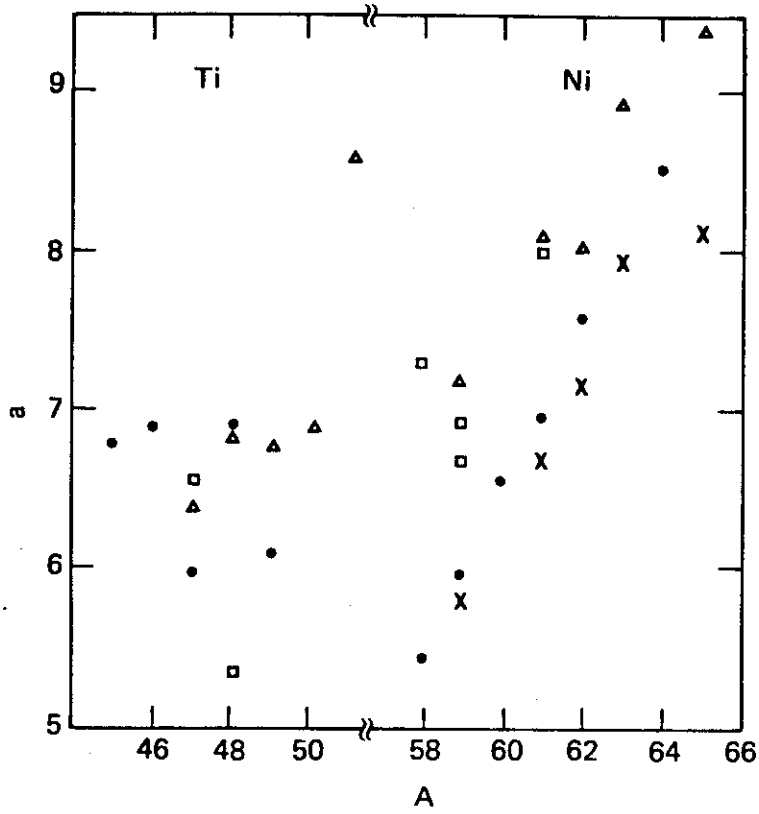

Fig. 1

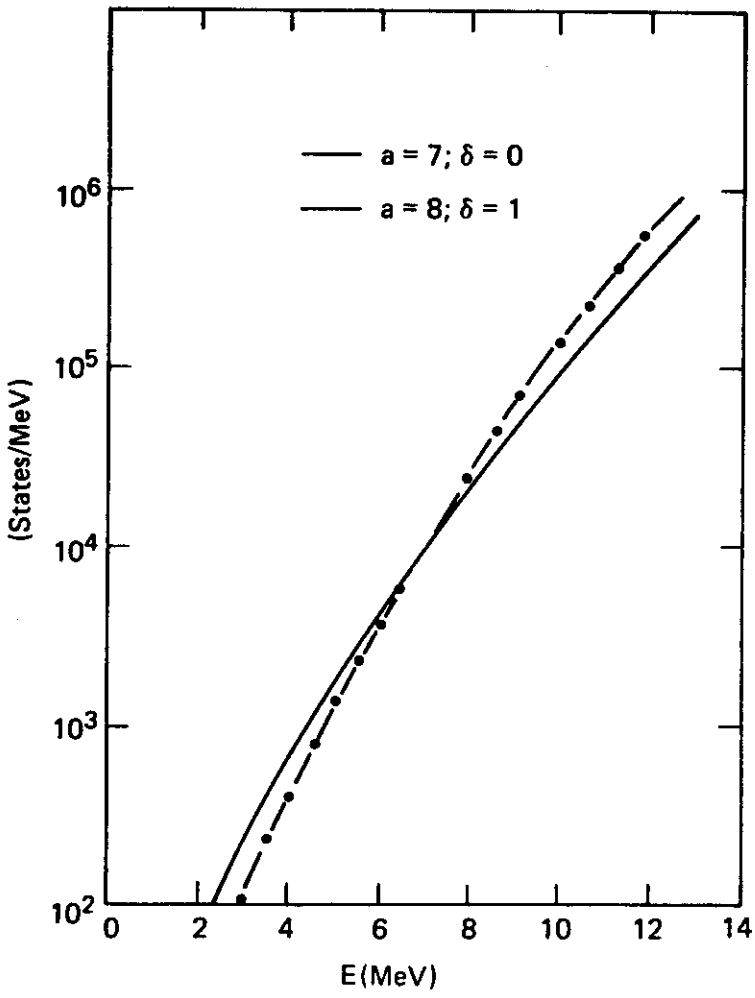

Fig. 2

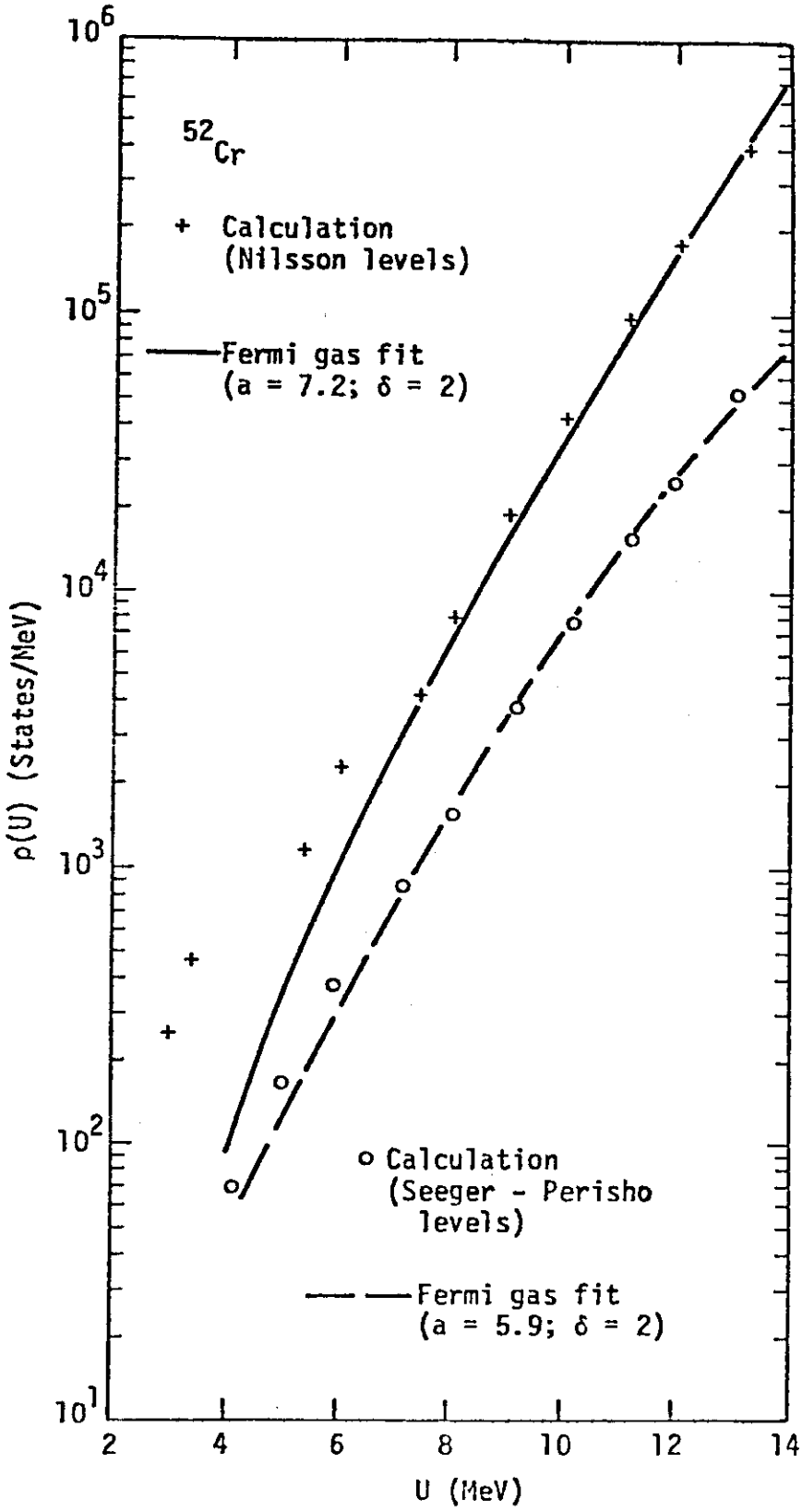
10^6
10^5
10^4
10^3
10^2
10^1
^{52}Cr
+ Calculation
(Nilsson levels)
Fermi gas fit
(a = 7.2; δ = 2)
o Calculation
(Seeger - Perisho
levels)
Fermi gas fit
(a = 5.9; δ = 2)
ρ(U) (States/MeV)
2
4
6
8
10
12
14
U (MeV)

Fig. 3

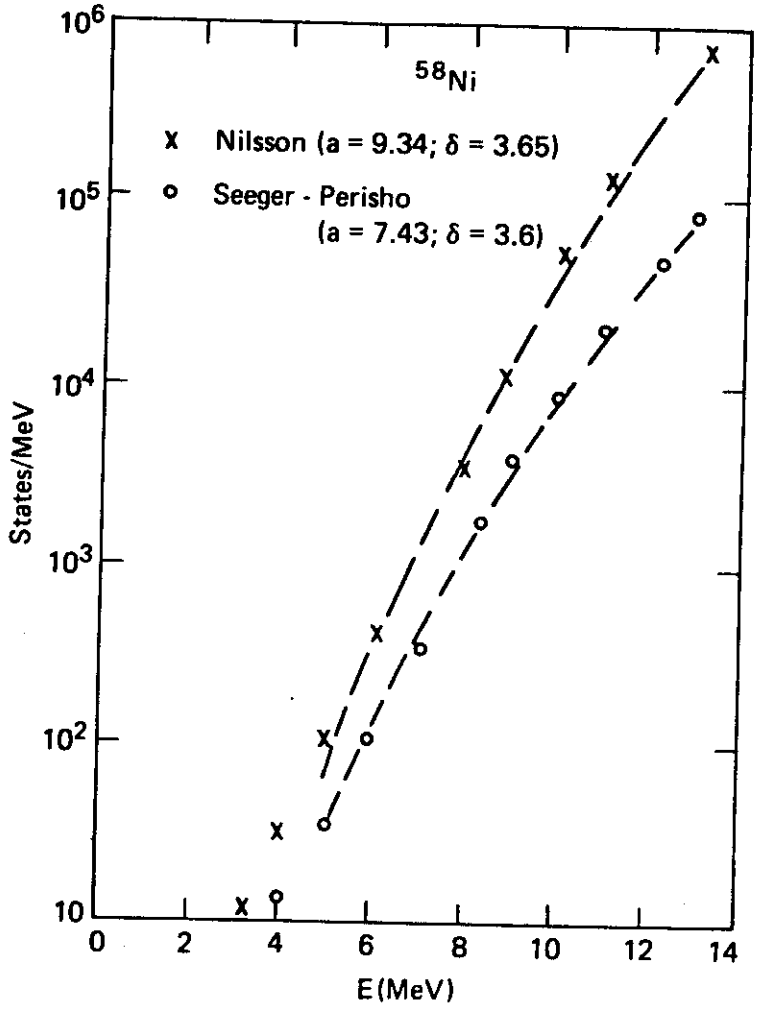
10^6
10^5
10^4
10^3
10^2
10
States/MeV
^{58}Ni
x Nilsson (a = 9.34; δ = 3.65)
o Seeger - Perisho
(a = 7.43; δ = 3.6)
0
2
4
6
8
10
12
14
E(MeV)

Fig. 4

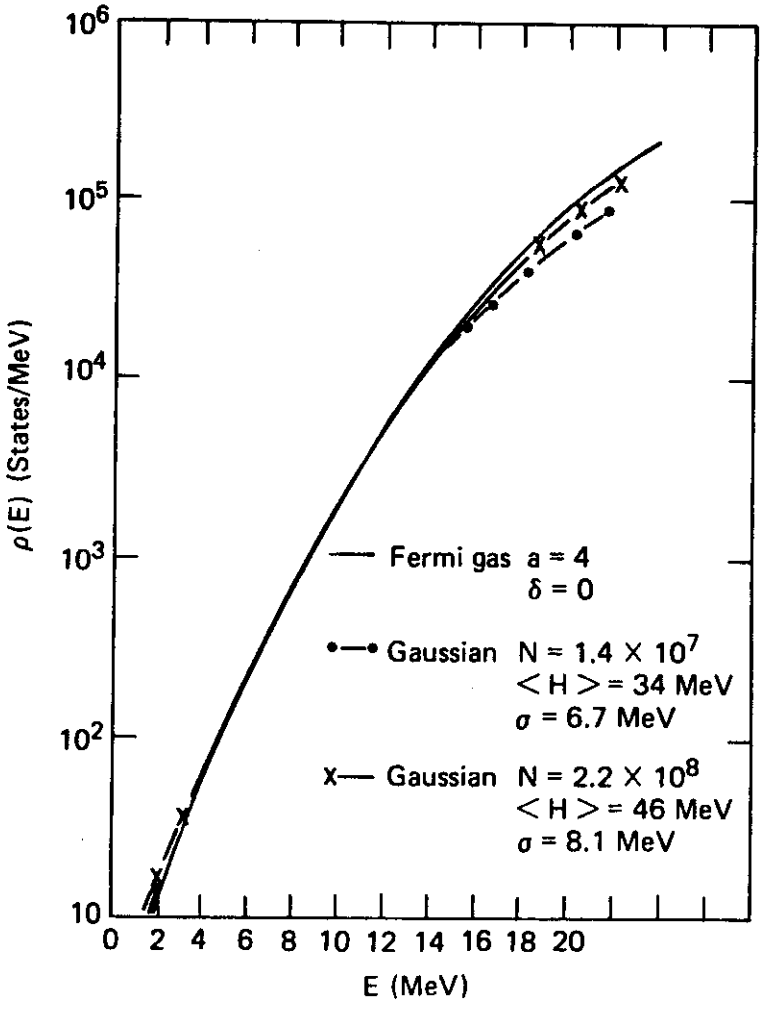
10^6
10^5
10^4
10^3
10^2
10
$\rho(E)$ (States/MeV)
0 2 4 6 8 10 12 14 16 18 20
E (MeV)
Fermi gas a = 4
δ = 0
Gaussian N = 1.4 X 10^7
< H > = 34 MeV
σ = 6.7 MeV
Gaussian N = 2.2 X 10^8
< H > = 46 MeV
σ = 8.1 MeV

Fig. 5

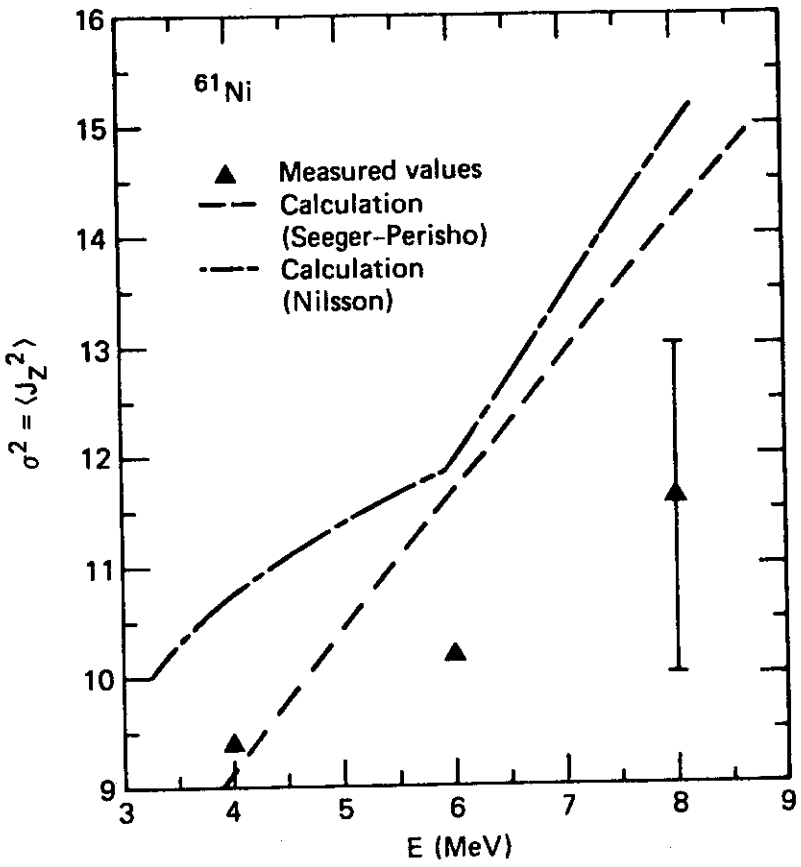
^{61}Ni
Measured values
Calculation
(Seeger-Perisho)
Calculation
(Nilsson)
$\sigma^2 = \langle J_Z^2 \rangle$
E (MeV)
16
15
14
13
12
11
10
9
3
4
5
6
7
8
9

Fig. 6

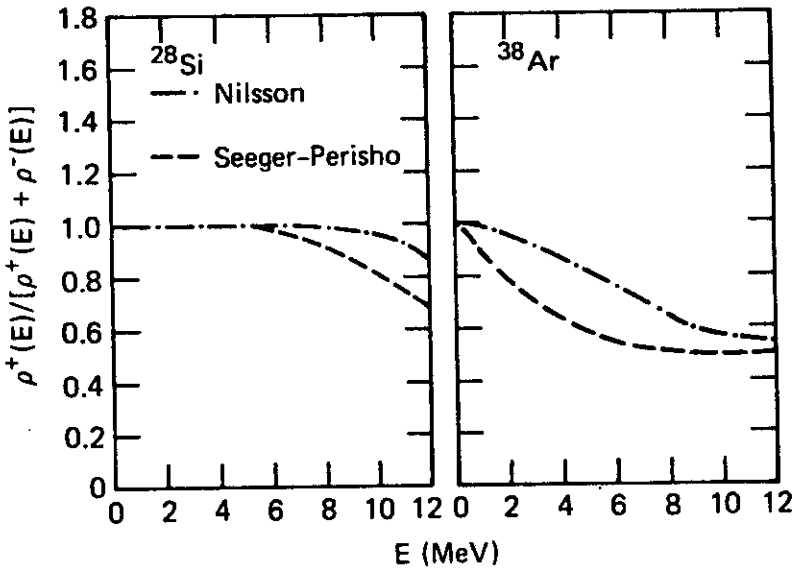
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
$\rho^+(E)/[\rho^+(E) + \rho^-(E)]$
^{28}Si
Nilsson
Seeger-Perisho
^{38}Ar
0 2 4 6 8 10 12
0 2 4 6 8 10 12
E (MeV)

Fig. 7